

VARIFLEX MANUAL EXAMPLE FILE

Version 1.0; July 16, 1999

Sample Test Runs

A. Overview of Sample Test Runs

The sample test runs were selected to illustrate various aspects of VARIFLEX. Since VARIFLEX is a shape driven code, reactions are selected that involve all combinations of differently shaped reactants [e.g., atom, linear top, or (a)symmetric top]. VARIFLEX does canonical and microcanonical reactions in completely consistent but different ways. Consequently both canonical and microcanonical runs are illustrated. Furthermore, VARIFLEX can treat both neutral and ionic reactions and examples are provided for both types of reactions. VARIFLEX can do RRKM calculations with and without Master Equation representations of pressure effects and this is illustrated. Finally, VARIFLEX can mix loose barrierless transition states and tight, barrier-dominated transition states in addition-elimination type reactions and these most complicated cases are also illustrated.

The following is a list of reactions involved in the test suite. If references are available for VARIFLEX studies of these reactions, they are included in the detailed descriptions given below. In many cases, VARIFLEX work on these reactions is not yet reported in the literature, or only preliminary reports are available. Work on these reactions will be the subject of future publications. In some cases there are minor differences from the results reported in the literature.

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|--------------------------------|---|
| 1. $\text{CH}_3 + \text{CH}_3$ | Canonical tests for a symmetric top + symmetric top reaction illustrating grid based and Monte Carlo integration schemes. Includes illustrations of geometry and frequency variation along the reaction path. |
| 2. $\text{NH}_2 + \text{NO}$ | Canonical tests for an asymmetric top + linear top reaction illustrating grid based and Monte Carlo integration schemes. |
| 3. $\text{CH} + \text{H}_2$ | Canonical tests for a linear top + linear top reaction illustrating grid based and Monte Carlo integration schemes. Also includes a comparable microcanonical test. |
| 4. $\text{CFH}_2 + \text{H}$ | Canonical tests for an asymmetric top + atom reaction illustrating grid based and Monte Carlo integration schemes. Also includes both radial and angular optimization of the pivot point location. |
| 5. $\text{CF}_3 + \text{H}$ | Canonical tests for a symmetric top + atom reaction illustrating grid based and Monte Carlo integration schemes. |
| 6. $\text{HCC} + \text{H}$ | Canonical tests for a linear top + atom reaction illustrating grid based and Monte Carlo integration schemes. |

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|---|---|
| 7. NC + NO | Pressure dependent E/J resolved tests for master equation, Troe, and modified strong collision modeling in a single product channel reaction. Includes illustration of Eigenvalue, Eigenvector, and Inversion based solutions to the master equation and PReacPQ and PCompPQ based reductions of E/J resolved rates to E resolved rates. Also illustrates effective and unified statistical evaluations of the E/J resolved number of states. |
| 8. NH + NO | Pressure dependent master equation based modeling of a multiple product channel reaction. Also illustrates tight barrier dominated transition state evaluations including tunneling corrections. |
| 9. C ₃ H ₆ + H | Pressure dependent master equation based modeling for a single product channel reaction employing inverse Laplace transform based determinations of the E resolved transition state partition functions. |
| 10. CH ₃ + OH | Pressure dependent master equation based modeling for a multiple product channel reaction employing inverse Laplace transform based determinations of the E resolved transition state partition functions. |
| 11. C ₆ H ₆ + Ag ⁺ | Radiative association kinetic modeling for an ion-molecule reaction including variational transition state theory, PST and low efficiency models for the kinetics. |
| 12. C ₆ H ₆ + Cr ⁺ | Collision induced dissociation modeling for an ion-molecule reaction. |
| 13. C ₄ NH ₅ + Fe ⁺ | Radiative association kinetic modeling for an ion-molecule reaction illustrating ion-dipole potential and multiple electronic states. |
| 14. C ₃ H ₆ O + C ₃ H ₆ OH ⁺ | Radiative association kinetic modeling for an ion-molecule reaction including strong-collision, master equation, and low efficiency models for the pressure dependence. |

Running a sample test run labelled vrfxtr1 will generally use some or all of the following input files, and produce some or all of the following output files

VARIFLEX I/O FILES

INPUT FILENAMES

| | | |
|-------------|---------|---------|
| vrfxtr1.dat | pot.dat | nej.dat |
|-------------|---------|---------|

OUTPUT FILENAMES

| | | | |
|-------------|---|---|----------------|
| vrfxtr1.out | vrfxtr1_cons.out vrfxtr1_flow.out vrfxtr1_tspf.out vrfxtr1_trate.out | vrfxtr1_erate.out vrfxtr1_intgl.out vrfxtr1_tspfr.out | vrfxtr1_pf.out |
|-------------|---|---|----------------|

B. Organization of the Sample Test Runs

Test runs for the same reaction are labeled by the reaction name, a suffix tr for test run, and a index n for which test run for the given reaction. For example, chh2tr3 is the third test run for the CH+H2 reaction. At the VARIFLEX anonymous ftp site, all test runs are in subdirectories of the /Examples directory. Each subdirectory is labeled by the reaction name (e.g., /CH+H2). Within each subdirectory, there is a save set of all input and output files associated with each test run. All the output files begin with the test run label of reaction, suffix tr, and index and end with .out (e. g, chh2tr2_tspfr.out or ch3ch3tr3.out). The number of saved output files varies from run to run. For each test run, there are two input files. One file called pot.dat is specific to the potential energy surface and is common to all test runs with the same potential energy surface. The second file contains no potential energy surface information but all input required to define the test run. That file is labeled by the reaction followed by the suffix tr followed by the run index followed by .dat (e.g., cf3htr2.dat). In addition to the saved set of input and output files, there is a "current" set of input files. These files are identical in content to the saved set of input files but have a file name that replaces the reaction name with "vrfx", as in vrfxtr2.dat for cf3htr2.dat. Execution of VARIFLEX with the "current" input file and pot.dat will produce output essentially identical to the saved set output.

Most reaction subdirectories have a potential subroutine. (Those that do not use the default potential energy surface supplied by VARIFLEX.) This potential subroutine has a file name that begins with Potcalc_ and ends with .f (e.g., Potcalc_cfh2h.f).

Each reaction subdirectory has several script files to assist in running VARIFLEX and comparing the output of the "current" input to the saved output. These script files are:

1. A "make" script file: Its label starts with make and ends with the reaction name (e.g., makech3ch3). It will construct the executable variflex.exe with the correct potential.
2. "run" script files: These script files are labeled by runvrfxtr followed by the index of the test run and will run the associated "current" input file (e.g., runvrfxtr3 will run vrfxtr3.dat). The script file runvrfxtrall will run all test runs in the reaction subdirectory.
3. A "diff" script file: The script file named difmaker will difference all the "current" output files with the saved set of output files and report any differences.
4. A "clean" script file: Successful runs with "current" input files create many output files that are all identical to the saved output files. The script cleanvrfxtr removes all "current" output files.
5. The main example directory also has the script files makeall (to make all the example exectuables), testall (to run all the samples and report any differences with the current saved set of ouput files), cleanall (to remove all "current" output files), maketestcleanall (to make, run, compare and clean all examples), and transferall (to make, run, compare, transfer the current output to the saved output, and clean all examples).

The time to solution for each test case is reported Table I for an IBM RISC/6000 Model 250 workstation with 32MB of memory. The timings are subdivided into five steps: reading input, constructing partition functions for conserved modes, constructing partition functions for transitional modes, constructing the rate, and collision induced dissociation modeling. The total time is also listed. Total time for all jobs exceeded 24 hours.

Table I. Timings in seconds (unless otherwise indicated) for all the test cases (see text for details).

| Test Run | Read | Cons. PF | Trans. PF | Rate | CID | Total |
|--------------|--------|----------|-----------|----------|-----------|-----------|
| ch3ch3tr1: | .1220 | .0020 | 28.40 | .00 | .0010 | 28.58 |
| ch3ch3tr2: | .0470 | .0020 | 28.00 | .00 | .0010 | 28.04 |
| ch3ch3tr3: | .0470 | .0010 | 8.96 | .00 | .0010 | 9.02 |
| ch3ch3tr4: | .0510 | .0010 | 77.00 | .00 | .0010 | 77.05 |
| nh2notr1: | .0340 | .0010 | 17.40 | .00 | .0010 | 17.49 |
| nh2notr2: | .0370 | .0010 | 103.00 | .00 | .0010 | 103.10 |
| nh2notr3: | .0410 | .0010 | 38.70 | .00 | .0000 | 38.78 |
| nh2notr4: | .0400 | .0020 | 48.70 | .00 | .0010 | 48.79 |
| chh2tr1: | .1770 | .0020 | 23.50 | .00 | .0000 | 23.67 |
| chh2tr2: | .1300 | .0020 | 173.00 | .00 | .0000 | 172.70 |
| chh2tr3: | .1270 | .0010 | 64.30 | .00 | .0000 | 64.41 |
| chh2tr4: | .1280 | .0010 | 99.50 | .00 | .0000 | 99.66 |
| chh2tr5: | .1280 | .0020 | 130.00 | .35 | .0000 | 130.90 |
| cfh2htr1: | .0600 | .0010 | 39.30 | .01 | .0000 | 39.35 |
| cf3htr1: | .0420 | .0020 | 1.80 | .01 | .0010 | 1.86 |
| cf3htr2: | .0280 | .0020 | 9.81 | .01 | .0010 | 9.85 |
| cf3htr3: | .0290 | .0010 | 76.10 | .01 | .0000 | 76.14 |
| cf3htr4: | .0300 | .0010 | 22.70 | .01 | .0000 | 22.70 |
| hcchtr1: | .0430 | .0010 | 1.99 | .01 | .0000 | 2.04 |
| hcchtr2: | .0300 | .0020 | 42.60 | .01 | .0000 | 42.59 |
| hcchtr3: | .0300 | .0020 | 3.99 | .01 | .0010 | 4.03 |
| ncnotr1: | .0760 | .0020 | 4960.00 | 6700.00 | .0010 | 11660.00 |
| ncnotr2: | .7020 | .0440 | 4940.00 | 4910.00 | .0010 | 9853.00 |
| ncnotr3: | .0720 | .0030 | 4940.00 | 17900.00 | .0010 | 22840.00 |
| ncnotr4: | .6560 | .0350 | 4940.00 | 4350.00 | .0010 | 9295.00 |
| ncnotr5: | .7160 | .0450 | 4940.00 | 99.30 | .0010 | 5044.00 |
| ncnotr6: | .0580 | .0020 | 4940.00 | 111.00 | .0010 | 5050.00 |
| ncnotr7: | .0570 | .0020 | 4940.00 | 6690.00 | .0010 | 11630.00 |
| ncnotr8: | .2400 | .0530 | 8530.00 | 4350.00 | .0000 | 12890.00 |
| nhnotr1: | .2900 | .0150 | 3600.00 | 7940.00 | .0010 | 11540.00 |
| c3h6htr1: | .1100 | .0040 | .00 | 252.00 | .0010 | 252.50 |
| ch3ohtr1: | .0530 | .0010 | .00 | 14300.00 | .0000 | 14260.00 |
| c6h6agr1: | .0440 | .0020 | 202.00 | 35.00 | .0010 | 236.80 |
| c6h6agr2: | .0410 | .0020 | 112.00 | 34.60 | .0010 | 146.50 |
| c6h6agr3: | .0340 | .0020 | .00 | 34.30 | .0010 | 34.33 |
| c6h6ctr1: | .0460 | .0020 | 781.00 | 1.15 | 1810.0000 | 2593.00 |
| c4nh5fetr1: | .0620 | .0020 | 2180.00 | 2500.00 | .0010 | 4679.00 |
| pacedimtr1: | .0580 | .0020 | 364.00 | 25.20 | .0010 | 388.90 |
| pacedimtr2: | .0580 | .0030 | 369.00 | 213.00 | .0010 | 582.70 |
| pacedimtr3: | .0450 | .0020 | .00 | 25.10 | .0010 | 25.17 |
| Total(sec.): | 4.8190 | .2540 | 51776.76 | 70471.11 | 1810.0260 | 124041.65 |
| (min.): | .0803 | .0042 | 862.95 | 1174.52 | 30.1671 | 2067.36 |
| (hr.): | .0013 | .0001 | 14.38 | 19.58 | .5028 | 34.46 |

C. Detailed Description of Sample Test Runs

C.1.2 Test run ch3ch3tr1 CH_3+CH_3 Products at low temperature

This sample run is for the canonical rate constant of the reaction CH_3+CH_3 products in the high pressure limit at 300K. It is an example of a symmetric top + symmetric top reaction. There are no pivot point displacements from the center of mass. The conserved frequencies vary with the center of mass separation (RdepVibP is selected). The geometry of the fragments at the asymptote is planar but along the section of the reaction path sampled is splayed (RdepGeoP is selected). The potential energy surface, conserved frequencies, and geometries along the reaction path are those used by Wardlaw and Marcus [*J. Chem. Phys.* **123**, 456 (1985)]. A numerical grid procedure is used (GridIntD is selected) and tests show that the parameters selected converge the rate constant to within about 1%. The results agree with the canonical rates in the above reference to within 10%, and to within 2% of the canonical rates in Pacey et al., [*J. Chem. Phys.* **321**, 654 (1987)] for nominally the same potential energy surface.

C.1.2 Test run ch3ch3tr2 CH_3+CH_3 Products at high temperature

This sample run is the same as ch3ch3tr1 except it is for a temperature of 2000K. Also, the splayed geometry corresponds to that appropriate for this temperature.

C.1.3 Test run ch3ch3tr3 CH_3+CH_3 Products at high temperature

This sample run is identical to ch3ch3tr2 except for the use of Monte Carlo integration instead of grid-based integration. A stratified Monte Carlo procedure is used (MonteCarloTD is selected with type = 2) and tests show that the parameters selected converge the rate constant to within about 10%. This Monte Carlo case makes about 75% fewer calls to the potential energy surface and thus is much faster.

C.1.4 Test run ch3ch3tr4 CH_3+CH_3 Products at moderately high temperature

This sample run is similar to ch3ch3tr1 but it is for a temperature of 1000 K and it illustrates the effect of pivot point displacements from the center of mass along the C_{3v} axis for both reactants. The results imply that modest changes in the displacement ($\sim 0.15 \text{ \AA}$) will minimize the rate constant to a value about $\sim 5\%$ lower than that for no displacement.

C.2.1 Test run nh2notr1

NH₂+NO Products

This sample run is for the canonical rate constant of the reaction NH₂+NO products in the high pressure limit at 300K and 2000K. It is an example of an asymmetric top + linear top reaction. There are no pivot point displacements from the center of mass. The potential energy surface is the default selection with a Morse form to the bonding potential and a Lennard Jones form for the non-bonding potential. While different in detail, the constructed potential is similar to that used by Diau and Smith [*J. Chem. Phys.* **123**, 456 (1985)]. A numerical grid procedure is used (GridIntD is selected) and tests show that the parameters selected converge the rate constant to within about 1%.

C.2.2 Test run nh2notr2

NH₂+NO Products at high temperature

This sample run is similar to nh2notr1 but is for only a temperature of 2000 K and it includes major pivot point displacements from the center of mass along the bond length of NO and along the C_{2v} axis of NH₂. Results indicate that major displacements along the NO axis are necessary to minimize the rate constant. Displacement variations along the NH₂ C_{2v} axis have a negligible effect.

C.2.3 Test run nh2notr3

NH₂+NO Products at high temperature

This run is identical to nh2notr2 except for the substitution of crude Monte Carlo integration for grid-based integration and the consideration of a few additional pivot points. A crude Monte Carlo procedure is used (MonteCarloTD is selected with type = 1) and tests show that the parameters selected converge the rate constant to within about 10%.

C.2.4 Test run nh2notr4

NH₂+NO Products at high temperature

This run is identical to nh2notr3 with the substitution of stratified for crude Monte Carlo integration. A stratified Monte Carlo procedure is used (MonteCarloTD is selected with type = 2) and tests show that the parameters selected converge the rate constant to within about 1%.

C.3.1 Test run chh2tr1 $\text{CH}+\text{H}_2$ Products

This sample run is for the canonical rate constant of the reaction $\text{CH}+\text{H}_2$ products in the high pressure limit for 300K and 2000K. It is an example of a linear top + linear top reaction. There are no pivot point displacements from the center of mass. The potential energy surface is that used by Wagner and Harding [*J. Chem. Phys.* **123**, 456 (1985)]. A numerical grid procedure is used (GridIntD is selected) and tests show that the parameters selected converge the rate constant to within about 1%.

C.3.2 Test run chh2tr2 $\text{CH}+\text{H}_2$ Products at high temperature

This sample run is similar to chh2tr1 but includes pivot point displacements from the center of mass in all allowable directions for both CH and H_2 (but with the symmetry of H_2 explicitly considered), and considers only a temperature of 2000 K. A numerical grid procedure is used (GridIntD is selected) and tests show that the parameters selected converge the rate constant to within about 1%. These parameters are different from those used in chh2tr1 where no pivot point displacement is used. Part of the difference is the loss of symmetry with displacements from the center of mass of H_2 . Part of the difference is a greater sensitivity to the details of the integrand variation in one of the angles. The results indicate that pivot point displacements do not minimize the rate constant at this temperature.

C.3.3 Test run chh2tr3 $\text{CH}+\text{H}_2$ Products

This test run is identical to chh2tr1 except for Monte Carlo integration instead of grid-based integration. A crude Monte Carlo procedure is used (MonteCarloTD is selected with type = 1) and tests show that the parameters selected converge the rate constant to within about 5% of the numerical grid-based result obtained in chh2tr1.

C.3.4 Test run chh2tr4 $\text{CH}+\text{H}_2$ Products

This test run is identical to chh2tr3 except a stratified, instead of crude, Monte Carlo integration is used. A stratified Monte Carlo procedure is used (MonteCarloTD is selected with type = 2) and tests show that the parameters selected converge the rate constant to within about 10% of the numerical grid-based result obtained in chh2tr1. This stratified run has 50% more Monte Carlo points than the crude run (2250 & 1500, respectively) but the results are not as accurate vis a vis the grid-based results. With relatively small ensembles, Monte Carlo predictions tend to fluctuate strongly with the ensemble size, regardless of the particular sampling method employed. Estimate of both accuracy and inherent statistical uncertainty (in the form of the root mean square deviation) are thus of limited utility.

C.3.5 Test run chh2tr5 $\text{CH}+\text{H}_2$ Products

This test run is a microcanonical test run which reproduces the canonical rate at 2000 K by employing a single TS dividing surface equivalent to the optimized dividing surface found in chh2tr2.

C.4.1 Test run cfh2htr1

CFH₂+H Products

This sample run is for the canonical rate constant of the reaction CFH₂+H products in the high pressure limit from 300K to 600K. It is an example of a highly asymmetric top + atom reaction. There are major pivot point displacements from the center of mass in both radial and angular directions. The potential energy surface is that developed by Harding [*J. Chem. Phys.* **123**, 456 (1985)]. A numerical grid procedure is used (GridIntD is selected) and tests show that the parameters selected converge the rate constant to within about 1%. The results indicate that major pivot point displacements are necessary to minimize the rate constant.

C.5.1 Test run cf3htr1

CF₃+H Products

This sample run is for the canonical rate constant of the reaction CF₃+H products in the high pressure limit from 300K to 2000K. It is an example of a symmetric top + atom reaction. There are no pivot point displacements from the center of mass. The potential energy surface is that developed by Harding [*J. Chem. Phys.* **123**, 456 (1985)]. A numerical grid procedure is used (GridIntD is selected) and tests show that the parameters selected converge the rate constant to within about 1%.

C.5.2 Test run cf3htr2

CF₃+H Products

This sample run is similar to cf3htr1 except it includes major pivot point displacements from the center of mass along the C_{3v} axis. The results indicate that major displacements of the pivot point are necessary to minimize the rate constant.

C.5.3 Test run cf3htr3

CF₃+H Products

This test run is identical to cf3htr2 except for Monte Carlo instead of grid-based integration. A crude Monte Carlo procedure is used (MonteCarloTD is selected with type = 1) and tests show that the parameters selected converge the rate constant to within about 10% and converge optimum pivot point displacements to about 0.1 Å.

C.5.4 Test run cf3htr4

CF₃+H Products

This test run is identical to cf3htr3 except for stratified instead of crude Monte Carlo integration. A stratified Monte Carlo procedure is used (MonteCarloTD is selected with type = 2) and tests show that the parameters selected converge the rate constant to within about 5% and converge optimum pivot point displacements to about 0.1 Å.

C.6.1 Test run hcchtr1

HCC+H Products

This sample run is for the canonical rate constant of the reaction HCC+H products in the high pressure limit from 300K to 2000K. It is an example of a linear top + atom reaction. There are major pivot point displacements from the center of mass along the bond axis. The potential energy surface is that developed by Harding [*J. Chem. Phys.* **123**, 456 (1985)]. A numerical grid procedure is used (GridIntD is selected) and tests show that the parameters selected converge the rate constant to within about 1%. The results indicate that major pivot point displacements are necessary to minimize the rate constant.

C.6.2 Test run hcchtr2

HCC+H Products

This test case is identical to hcchtr1 with the substitution of crude Monte Carlo for grid-based integration. A crude Monte Carlo procedure is used (MonteCarloTD is selected with type = 1) and tests show that the parameters selected converge the rate constant to within about 10%.

C.6.3 Test run hcchtr3

HCC+H Products

This test case is identical to hcchtr2 with the substitution of stratified for crude Monte Carlo integration. A stratified Monte Carlo procedure is used (MonteCarloTD is selected with type = 1) and tests show that the parameters selected converge the rate constant to within about 10%.

C.7.1 Test run ncnotr1

NC+NO NCNO

This sample run is a master equation based calculation of the temperature and pressure dependence of the rate constant for the reaction $\text{NC} + \text{NO} \rightarrow \text{NCNO}$ from 102 to 740 K and 1 to 10^5 torr [cf., S. J. Klippenstein, D. L. Yang, T. Yu, S. Kristyan, M. C. Lin, S. H. Robertson, *J. Phys. Chem. A*, **102**, 6973, (1998)]. It illustrates the data input for an effective number of states calculation and for contributions to the TS from multiple electronic states. For the first effective state (the outer TS) the pivot points are taken to lie at the centers-of-mass of NC and of NO. For the second effective state (the inner TS) the pivot points are assumed to lie at the two bonding atoms C in CN and N in NO. The potential energy surface is a revised version of the model potential developed by Klippenstein and Marcus [*J. Phys. Chem.* **89**, 4761 (1988)]. The master equation is solved with a matrix inversion based procedure using the method of Smith and Gilbert [*Int. J. Chem. Kinet.* **20**, 307, 979 (1988)] to reduce the E/J resolved rates to E resolved rates.

C.7.2 Test run ncnotr2

NC+NO NCNO

This case is identical to ncnotr1 except for the solution of the master equation with a eigenvalue based procedure. The difference between these results at the lower temperatures and those from ncnotr1 is indicative of numerical failures in the eigenvalue solution.

C.7.3 Test run ncnotr3

NC+NO NCNO

This case is identical to ncnotr1 except for the solution of the master equation with a eigenvector based procedure.

C.7.4 Test run ncnotr4

NC+NO NCNO

This case is identical to ncnotr1 except for the use of just the Boltzman probability for the complex for the J averaging in the reduction to 1-dimension in the master equation (**PCompPQ** vs **PReacPQ**).

C.7.5 Test run ncnotr5 NC+NO NCNO

This case is identical to ncnotr1 except for the replacement of the master equation with a modified strong collision analysis.

C.7.6 Test run ncnotr6 NC+NO NCNO

This case is identical to ncnotr1 except for the replacement of the master equation with a Troe style analysis.

C.7.7 Test run ncnotr7 NC+NO NCNO

This case is identical to ncnotr1 except for the replacement of the effective number of states evaluation with the minimum over the two transition state regions.

C.7.8 Test run ncnotr8 NC+NO NCNO

This case is identical to ncnotr1 except for the replacement of the effective number of states evaluation with the unified statistical analysis of Miller [*J. Chem. Phys.* **65**, 2216 (1976)].

C.8.1 Test run nhnotr1

NH+NO Products

This sample run is a master equation based calculation of the temperature and pressure dependence of the rate constant for the reaction $\text{NH} + \text{NO} \rightarrow \text{HNNO} \rightarrow \text{H} + \text{N}_2\text{O}$ and $\text{N}_2 + \text{OH}$ from 200 to 3500 K, and 1 to 10^6 torr, with exponential down parameter (ρ) of 100, 400, and 1600 cm^{-1} . It illustrates the data input for 4 channels, for variable and tight transition states, for an effective number of states calculation, and for contributions to the TS from multiple electronic states. The potential energy surface [unpublished Klippenstein and Lin] employs a minor variation to the default potential and illustrates the input format for both the interpolated and extrapolated potential forms. The master equation is solved with a matrix inversion based procedure using the method of Smith and Gilbert [*Int. J. Chem. Kinet.* **20**, 307, 979 (1988)] to reduce the E/J resolved rates to E resolved rates.

C.9.1 Test run c3h6htr1

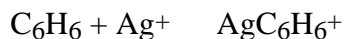
$\text{C}_3\text{H}_6 + \text{H}$ Products

Pressure dependent master equation based modeling for a single product channel reaction employing inverse Laplace transform based determinations of the E resolved transition state partition functions.

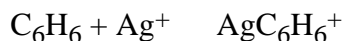
C.10.1 Test run ch3ohtr1

CH₃ + OH Products

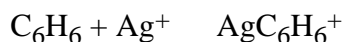
Pressure dependent master equation based modeling for a multiple (2) product channel reaction employing inverse Laplace transform based determinations of the E resolved transition state partition functions.

C.11.1 Test run c6h6agtr1

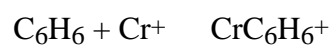
This sample run is for the association rate constant of the reaction $\text{C}_6\text{H}_6 + \text{Ag}^+ \rightarrow \text{AgC}_6\text{H}_6^+$ at 300K and neutral pressures from 1×10^{-9} to 9.3×10^{-7} Torr [cf., Y.-P. Ho, Y.-C. Yang, S. J. Klippenstein, and R. C. Dunbar, *J. Phys. Chem.* **101**, 3338, (1997)]. It is calculated assuming thermal reactants employing a center-of-mass reaction coordinate in EJ resolved variational transition state theory evaluations (VRC). A single binding energy of 11,000 cm⁻¹ is used. The potential energy function is the built-in ion-induced dipole potential. The strong-collision assumption is made for collisional stabilization of the complex. Radiative stabilization is calculated from input values of vibrational frequencies and intensities of the complex.

C.11.2 Test run c6h6agtr2

This sample run is identical to c6h6agtr1 except for the use of Phase Space Theory in place of the VRC calculation.

C.11.3 Test run c6h6agtr3

This sample run is identical to c6h6agtr1 except for the use of the low-efficiency approximation.

C.12.1 Test run c6h6crtr1

Collision induced dissociation modeling for an ion-molecule reaction.

C.13.1 Test run c4nh5fetr1 $\text{C}_4\text{NH}_5 + \text{Fe}^+ \rightarrow \text{FeC}_4\text{NH}_5^+$

Radiative association kinetic modeling for an ion-molecule reaction illustrating ion-dipole potential and multiple electronic states.

C.14.1 Test run pacedimtr1 $\text{C}_3\text{H}_6\text{O} + \text{C}_3\text{H}_6\text{O} \text{H}^+ \rightarrow \text{C}_3\text{H}_6\text{O} \cdot \text{C}_3\text{H}_6\text{OH}^+$

This sample run is for the association rate constant of the reaction $\text{C}_3\text{H}_6\text{O} + \text{C}_3\text{H}_6\text{OH}^+ \rightarrow \text{C}_3\text{H}_6\text{O} \cdot \text{C}_3\text{H}_6\text{OH}^+$ at 300.7 K and neutral pressures from 1×10^{-8} to 1.0 Torr [cf., S. J. Klippenstein, Y.-C. Yang, V. Ryzhov, and R. C. Dunbar, *J. Chem. Phys.* **104**, 4502 (1996)] . It is calculated assuming thermal reactants employing a center-of-mass reaction coordinate in EJ resolved variational transition state theory evaluations (VRC). A single binding energy of 10493 cm^{-1} is used. The potential energy function is the built-in potential with an ion-induced dipole term and an ion-dipole term. The strong-collision assumption is made for collisional stabilization of the complex. Radiative stabilization is calculated from input values of vibrational frequencies and intensities of the complex.

C.14.2 Test run pacedimtr2 $\text{C}_3\text{H}_6\text{O} + \text{C}_3\text{H}_6\text{OH}^+ \rightarrow \text{C}_3\text{H}_6\text{O} \cdot \text{C}_3\text{H}_6\text{OH}^+$

This sample run is identical to pacedimtr1 except for the use of a one-dimensional master-equation in place of the strong collision assumption for the collisional stabilization of the complex.

C.14.3 Test run pacedimtr3 $\text{C}_3\text{H}_6\text{O} + \text{C}_3\text{H}_6\text{OH}^+ \rightarrow \text{C}_3\text{H}_6\text{O} \cdot \text{C}_3\text{H}_6\text{OH}^+$

This sample run is identical to pacedimtr1 except for the use of the low efficiency approximation.